

Calculation of Distillation Refining of a Substance Containing Low and Highly Volatile Impurities

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Abstract—This paper considers the distillation refining of a material containing highly volatile and low-volatile impurities and demonstrates the possibility of evaluating the fraction of residue, g_r , during the removal of the highly volatile impurity and the degree of subsequent distillation, g_c , necessary for achieving a predetermined decrease in impurity concentrations at a predetermined product yield and known separation factors. Examples are presented for the distillation in real host–impurity systems: Ga–(Pb,Al), Be–(Al,Fe), and Cr–(Si,Fe).

Keywords: distillation, degree of distillation

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INTRODUCTION

Distillation is among the main processes for the preparation of high-purity substances, which has aroused considerable interest in the theory of the process [1–9]. Distillation refining can be described using the following simple equations [7–9]:

$$\frac{C_c}{C_0} = \frac{1 - (1 - g)^\beta}{g}, \quad (1)$$

$$\frac{C_r}{C_0} = g_r^{\beta-1}, \quad (2)$$

where C_c and C_r are the impurity concentrations in the condensate and residue, respectively; C_0 is the initial impurity concentration; g is the degree of distillation (the ratio of the mass of the condensate to the initial mass of the material being distilled); g_r is the mass fraction of the residue (the ratio of the mass of the residue to the initial mass of the material being distilled); and β is the separation factor (the ratio of the impurity concentration in the vapor forming from the liquid phase to that in the liquid phase).

A starting material to be refined often contains two difficult-to-remove impurities (with β values near unity): highly volatile ($\beta > 1$) and low-volatile ($\beta < 1$). Examples of such materials among inorganic substances are presented in Table 1. (Such examples can also be indicated for organic substances.)

In refining such materials, sequential distillation in two modes is needed to remove both impurities: (1) driving off a portion of the substance at temperature

T_1 , until the fraction of the residue is g_r , for refining the residue to remove the highly volatile impurity and (2) subsequent distillation at temperature T_2 to a degree of distillation g_c in order to remove the low-volatile impurity from the condensate (the reverse order of the steps is also possible). Note that the removal of the highly volatile impurity from the residue in the first refining step is accompanied by an increase in the concentration of the low-volatile impurity, and the preparation of a condensate free of the low-volatile impurity in the second refining step is accompanied by an increase in the concentration of the highly volatile impurity in the condensate. It is therefore interesting to calculate the fraction of the residue, g_r , in the first distillation step and the degree of distillation, g_c , necessary for achieving a predetermined reduction in impurity concentration at a predetermined, economically reasonable product yield and known separation factors.

THEORY

The problem can be solved using Eqs. (1) and (2). Let the initial concentrations of the highly volatile and low-volatile impurities be C_{01} and C_{02} , respectively, and the separation factors for these impurities be β_{r1} and β_{r2} in the first step (stripping) and β_{c1} and β_{c2} in the second step (fractionation). Using Eq. (2), we obtain for the first distillation step (stripping)

$$\frac{C_{r1}}{C_{01}} = g_r^{\beta_{r1}-1}, \quad (3)$$

Table 1. Examples of refinable substances containing highly and low volatile impurities

Host	wt % impurity		Ref.
	highly volatile	low volatile	
Be	[Al] ~ 0.1	[Fe] ~ 0.1	[6]
Ga	[Pb] ~ 10 ⁻²	[Al] ~ 10 ⁻²	[10]
Cr	[Si] ~ 10 ⁻³	[Fe] ~ 10 ⁻³	[11]
Te	[Se] ~ 10 ⁻²	[Al] ~ 10 ⁻²	[12]
Tm	[Ca] ~ 10 ⁻²	[Cu] ~ 10 ⁻²	[13]

$$\frac{C_{r2}}{C_{02}} = g_r^{\beta_{r2}-1}, \quad (4)$$

where C_{r1} and C_{r2} are the concentrations of the highly volatile and low-volatile impurities, respectively, in the residue after the first distillation step and g_r is the fraction of the residue in the first refining step.

Using C_{r1} and C_{r2} as the initial impurity concentrations in the second refining step (fractionation), we obtain from Eq. (1)

$$\frac{C_{c1}}{C_{01}} = g_r^{\beta_{c1}-1} \frac{1 - (1 - g_c)^{\beta_{c1}}}{g_c}, \quad (5)$$

$$\frac{C_{c2}}{C_{02}} = g_r^{\beta_{c2}-1} \frac{1 - (1 - g_c)^{\beta_{c2}}}{g_c}, \quad (6)$$

where C_{c1} and C_{c2} are the concentrations of the highly volatile and low-volatile impurities, respectively, in the condensate in the second step.

Dividing Eq. (5) by Eq. (6), we obtain

$$g_r^{\beta_{r1}-\beta_{r2}} = K \frac{1 - (1 - g_c)^{\beta_{c2}}}{1 - (1 - g_c)^{\beta_{c1}}}, \quad (7)$$

where $K = \frac{C_{c1}}{C_{01}} / \frac{C_{c2}}{C_{02}}$.

From Eq. (7) and the equation

$$g = g_r g_c, \quad (8)$$

(where $g < g_r$ and $g < g_c$), we obtain a system of two equations, (7) and (8), in two unknowns, g_r and g_c

(with C_{c1}/C_{01} , C_{c2}/C_{02} , g , β_{r1} , β_{r2} , β_{c1} , and β_{c2} as parameters). This system of equations can be solved numerically.

It is easy to show that Eqs. (7) and (8) describe as well the process in which the sequence of two refining steps (stripping and distillation) is reversed.

DISCUSSION

The following particular cases can be distinguished:

(a) a process with a uniform reduction in the concentrations of both impurities ($C_{c1}/C_{01} = C_{c2}/C_{02}$), that is, with $K = 1$; and

(b) a process in which $C_{01} \neq C_{02}$, but the impurity concentrations in the product are equal ($C_{c1} = C_{c2}$), so that $K = C_{02}/C_{01}$.

As an example, consider a process in which both distillation steps are performed at the same temperature T (at which $\beta_{r1} = \beta_{c1} = \beta_1$ and $\beta_{r2} = \beta_{c2} = \beta_2$), with a uniform decrease in the concentrations of both impurities ($K = 1$). Equation (7) then simplifies to

$$g_r^{\beta_1-\beta_2} = \frac{1 - (1 - g_c)^{\beta_2}}{1 - (1 - g_c)^{\beta_1}}. \quad (9)$$

Taking into account Eq. (8), we obtain

$$g^{\beta_1-\beta_2} = g_c^{\beta_1-\beta_2} \frac{1 - (1 - g_c)^{\beta_2}}{1 - (1 - g_c)^{\beta_1}}. \quad (10)$$

The sought parameters of this process ($K = 1$) in real systems are listed in Table 2, obtained using Eqs. (8) and (10). As the separation factors β_1 and β_2 , we used the ideal separation factor as the ratio of the vapor pressures of pure components [14]: impurity and host. (Using Eq. (10), we numerically found g_c , then chose $g < g_c$, and calculated g_r using Eq. (9) and C_{c1}/C_{01} using Eq. (3)).

Table 2 provides an idea of $g_r(g)$ and $g_c(g)$ dependences. In the Ga-(Pb,Al) system, g_r changes slightly and g_c changes more significantly as the yield g rises from 0.6 to 0.8. This is accompanied by a decrease in purification efficiency: each impurity concentration drops by a factor of 3 at $g = 0.6$ and by just a factor of 2

Table 2. Calculation of g_r , g_c , and degree of purification $C_{01}/C_{c1} = C_{02}/C_{c2}$ for a number of host-impurity systems in processes with uniform removal of both impurities ($K = 1$) at temperature T

System	T , K	Initial parameters			Calculation results		
		β_1	β_2	g	g_r	g_c	C_{01}/C_{c1}
Ga-(Pb,Al)	1600	35	0.3	0.6	0.97	0.62	3
				0.8	0.98	0.82	2
Be-(Al,Fe)	1800	2.3	0.1	0.3	0.40	0.75	3
Cr-(Si,Fe)	1800	1.7	0.4	0.3	0.50	0.60	1.6

at $g = 0.8$. A marked increase in the purification efficiency of this system can be reached at a significant decrease in the final yield g . At the same time, it is obvious that investigation of the $g_r(g)$ and $g_c(g)$ dependences in the Be–(Al,Fe) and Cr–(Si,Fe) systems in the problem under consideration (with equal degrees of removal of the two impurities) is of no practical interest, because a relatively low degree of purification in these systems (by a factor of 3 and 1.6, respectively) is reached at a rather low total yield: $g = 0.3$. (In the Te–(Se,Al) and Tm–(Ca,Cu) systems, a high degree of purification can be reached at $g_r \approx g_c \approx 1$, because the separation factor in these systems differs drastically from unity [14].)

Thus, the proposed calculation procedure for the distillation of a substance containing two impurities (highly volatile and low-volatile) makes it possible to evaluate the fraction of the residue, g_r , during the removal of the highly volatile impurity and the degree of subsequent distillation, g_c , necessary for achieving a predetermined decrease in impurity concentrations at various product yields g and to study $g_r(g)$ and $g_c(g)$ dependences. Such calculation is useful for optimizing the distillation refining of individual substances.

CONCLUSIONS

We have considered the distillation refining of a material containing highly volatile and low-volatile impurities and demonstrated the possibility of evaluating the fraction of residue, g_r , during the removal of the highly volatile impurity and the degree of subsequent distillation, g_c , necessary for achieving a predetermined decrease in impurity concentrations at a predetermined product yield and known separation factors, using the system of equations (7) and (8), which can be solved numerically.

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